

Binding Energy Evaluation of a Nano Dot as a Function of Dot Radius at Different Concentrations

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(Received on: July 16, 2013)

ABSTRACT

We have evaluated the binding energy of spherical GaAs/Ga_{1-x}InSb quantum dot as a function of dot radius at different composition x using the theoretical formalism of T. Prem Kumar *et al.* (2011). We observed that binding energy decreases with increase of dot radius with fixed concentration x . we also observed that if dot radius is kept fixed then binding energy increases with composition x . These observations are consentient with observations of other theoretical workers.

Keywords: Nano dot, Quantum Well, Variational quartz, effective mass approximation, Shallow impurity, molecular beam epitaxy.

1. INTRODUCTION

Recent advance is crystal growth techniques like fine line lithography, metal organic chemical vapor deposition (MOCVS) and molecular beam epitaxy (MBE) have made possible the fabrication of low dimensional semiconductor structures such as quantum well, quantum wires and quantum dots¹⁻⁵. A quantum well (QW) is formed when a thin layer of lower band gap semiconductor is sandwiched between two longer of higher band gap semiconductor^{6,7}.

In the quantum well structure, electrical and optical properties of the semiconductor are totally different from those of the both material due to quantum effect^{8,9}. Due to modulation doping in QW structure, carriers are separated from ionized impurity. This increases the mobility of carrier due to reduced ionized impurity scattering. The carrier concentration in QW is high and the coulomb scattering is also reduced with sufficient thickness of space layer¹⁰.

Theoretical calculations for binding energy of the ground state of GaAs QW's

infinite quantum well wires¹¹ (QWW's) and quantum dots (Q'D's)¹² have been performed. Their studies show that for an infinite confinement potential the binding energy increases as the finite dimension (length or radius) is reduced. On the other hand for finite confinement potential the binding energy increases up to maximum and then begins to decrease. It has also been observed in the case of donor doped QW's and infinite QW's¹¹ that the binding energy is maximum when the impurity is located at the centre of the structure and decreases for position close to the edges. It has also been anticipated that the semiconductor quantum structure with zero dimension such as GaAlAs/GaAs nanostructure will show discrete electronic states because of electronic confinement.¹³ These impurities play a very important role in optical and transport phenomenon at low temperature. The binding energy and density of states of shallow impurities in cubic¹⁴ and spherical quantum dot¹⁵ have been calculated as a function of dot size. These studies indicate that addition of impurities can change the property of any quantum devices drastically.

Using the variational method, Porras– Montenegro¹⁶ studied a hydrogenic impurity in spherical QD systems with both finite and infinite barriers. They calculated the binding energy of the impurities increases and for finite barrier the increase is maximum at a poured and then sharply decreases. They also observed that binding energy increases with the reduction of dot size¹⁷. Very recently, T. Prem Kumar *et al.*¹⁸ have performed a calculation for binding energy of donor impurity in GaAs placed at the curve. They observed that the binding energy decreases as dot size increases. They

also observed that increase of donor binding energy when the variation of construction is included for all dot size.

In this paper, following the same procedure adopted by T. Prem Kumar *et al.*¹⁸ we have evaluated the binding energy as a function of dot size for different concentrations. Our theoretically evaluated result shows that binding energy decreases with increase of dot radius with fixed concentration. In another calculation, binding energy of quantum dots increases linearly with concentration x with fixed dot radius. These observations are compared with other theoretical workers¹⁹⁻²¹.

2. MATHEMATICAL FORMULA USED IN THE EVALUATION.

The Hamiltonian of a single hydrogenic shallow donor impurity in the effective mass approximation for spherical GaAs quantum dot is given by

$$H = \frac{-\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{\epsilon_o r} + V_D(r) \quad (1)$$

Where ϵ_o is the static dielectric constant of GaAs

$$V_D(\vec{r}_j) = \frac{V_o r^2}{R^2} \text{ for } |r| \leq R$$

$$V_D(|\vec{r}_j|) = V_o \text{ for } |r| > R$$

R is the dot radius.

V_o is the barrier height of the periodic dot given by

$$V_D(\vec{r}) = Q_C \Delta E_g(x)$$

Q_C is the conduction band off such parameter, which is taken to be 0.65.¹²

ΔE_g is the band gap difference between GaAs and $\text{Ga}_x\text{In}_{1-x}\text{Sb}$ which is given by¹⁹

$$\Delta E_g(x) = 0.235 + 1.653x + 0.431x^2 \text{ eV} \quad (2)$$

The units of length and energy used throughout the paper are the Bore radius R^* and effective Rydberg Ry^*

$$R^* = \hbar^2 \epsilon_o / m^* e^2$$

$$Ry^* = m^* e^4 / 2 \epsilon_o^2 \hbar^2$$

ϵ_o is the dielectric constant and m^* is the effective mass of electron in conduction band minimum of GaAs with values $R^* = 103.7 \text{ \AA}$ and $Ry^* = 5.29 \text{ meV}$

By using above units, Hamiltonian given in equation (1) assumes the form

$$H = -\nabla^2 - \frac{2}{r} + V(r) \quad (3)$$

Here, one has used a donor impurity in quantum dot of GaAs. Since an exact solution of the Hamiltonian in equation (1) is not possible, a variational method has been adopted.

The following wave functions are used to obtain the lowest state energies.

$$\psi = \begin{cases} A \frac{\sin Kr}{r} & r \leq R \\ B \exp(-K_2 r) & r \geq R \end{cases} \quad (4)$$

where A and B are the normalization constants. Hence

$$k_1 = \sqrt{\frac{2m^* E}{\hbar^2}} \quad (5)$$

$$k_2 = \sqrt{\frac{2m^* (E - V)}{\hbar^2}}$$

For finite dot and with inclusion of impurity potential in the Hamiltonian, one uses the following trial wave function for the ground state with impurity present.

$$\psi = \begin{cases} N_1 \frac{\sin K_1 r}{r} \exp(-\beta_1 r) & r \leq R \\ N_2 \exp(-K_2 r) \exp(-\beta_1 r) & r \geq R \end{cases} \quad (6)$$

Where β_1 is the variational parameter and N_1 and N_2 are normalization constants. The ionization energy is given by

$$E_{\text{ion}} = E_{\text{sub}} - \langle H \rangle_{\text{min}} \quad (7)$$

Where E_{sub} is the lowest sub band energy

$$E_{\text{sub}} = \frac{\hbar^2 k^2}{2m^*} \quad (8)$$

$$\text{where, } k = \frac{\pi}{R}$$

3. DISCUSSION OF RESULTS

In this paper, using the theoretical formulation of T. Prem Kumar *et al.*¹⁸, we have evaluated the donor binding energy of the spherical quantum nano dot $\text{GaAs/Ga}_{1-x}\text{In}_x\text{Sb}$ as a function of dot radius with different composition. The work has been performed using a variational ansatz within the effective mass approximation. The evaluated results are shown in table T₁ to table T₅. In table T₁, we have shown the evaluated results of binding energy of spherical $\text{GaAs/Ga}_{1-x}\text{In}_x\text{Sb}$ quantum dot as a function of dot radius (\AA) for different composition x starting with x=0.1, 0.2, 0.3, 0.4 and 0.5. Our theoretically evaluated results show that binding energy decreases

with the increase of dot radius keeping composition x fixed. The binding energy is large for small dot radius and for $x=0.1$. In table T₂, we repeated the calculations for quantum dot size ($R < 100 \text{ \AA}$). Here again we observed the similar trend. The binding energy decreases with increase of dot radius for all the composites $x=0.1$ to 0.5 . In table T₃, we have presented the theoretically evaluated results of binding energy of quantum dot as a function of concentration x for fixed value of dot radius $R=80 \text{ \AA}$. Here the binding energy increases as a function of composition x . The increase is linearly with respect to the composition. We repeated the

same calculation for another value of dot radius $R=150 \text{ \AA}$. Here again, we noticed the similar observation of increase of binding energy as a function of composition x . However, the magnitude of the binding energy is lower at $R=150 \text{ \AA}$ than to $R=80 \text{ \AA}$ for $x=0.1$ to $x=0.8$. The results are shown in table T₄. In table T₅, we have given the values of barrier height $V(Ry^*)$, energy gap parameter $E_g(Ry^*)$ for different concentration used in the calculation of binding energy of spherical quantum dot GaAs/Ga_{1-x}In_xSb. Some recent²²⁻²⁵ calculations on quantum dot also reveal the similar type of observers.

Table T₁

An evaluated results of binding energy of spherical GaAs/Ga_{1-x}In_xSb quantum dot as a function of the dot radius for different concentration x

Dot Radius (\AA)	Binding Energy (Ry^*)				
	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$
50	58.24	52.78	50.22	49.58	48.27
100	40.56	39.29	37.12	36.19	35.86
150	28.24	26.15	25.54	24.99	23.18
200	23.16	20.58	19.18	18.75	17.59
300	14.44	13.29	12.86	11.59	10.86
400	12.18	11.43	10.75	10.86	10.22
500	11.56	10.27	9.86	9.75	9.67
600	10.22	9.86	9.22	9.10	9.02
700	9.58	9.05	8.89	8.78	8.88
800	8.72	8.88	8.25	8.16	8.22
900	8.56	8.27	7.86	7.77	7.89
1000	7.85	7.58	7.42	7.18	7.22

Table T₂

An evaluated results of binding energy of spherical GaAs/Ga_{1-x}In_xSb quantum dot as a function of dot size (quantum level) for different concentration x

Dot Radius (A ^o)	Binding Energy (Ry*)				
	$x=0.1$	$x=0.2$	$x=0.3$	$x=0.4$	$x=0.5$
5	58.24	52.78	50.22	49.58	48.27
10	50.16	49.44	48.52	47.29	46.55
15	46.10	45.05	44.36	46.58	45.17
20	41.84	40.72	40.12	41.29	42.27
25	36.13	35.58	34.86	35.86	36.15
30	30.29	29.34	30.22	31.25	32.22
35	26.52	25.16	24.98	25.18	26.48
40	28.27	26.22	25.26	26.27	27.15
45	32.38	27.18	27.54	28.15	28.46
50	34.58	28.59	28.22	29.00	29.52
60	36.42	29.14	29.54	29.82	30.18
70	37.12	30.27	30.48	30.50	31.29
80	38.56	31.58	32.24	31.27	32.00
90	39.29	32.29	33.16	32.54	32.58
100	40.16	33.54	33.86	33.33	33.17

Table T₃

An evaluated results of binding energy of spherical GaAs/Ga_{1-x}In_xSb quantum dot as a function of different constants for parameter dot radius R=80A^o.

x	Binding energy (Ry*) (R=80A ^o)
0.10	10.27
0.15	11.56
0.20	12.82
0.25	13.54
0.30	15.22
0.35	20.16
0.40	22.29
0.45	24.50
0.50	26.86
0.55	27.42
0.60	28.55
0.65	29.29
0.70	30.48
0.80	32.27

Table T₄

An evaluated results of binding energy of spherical GaAs/Ga_{1-x}In_xSb quantum dot as a function of different constants for parameter dot radius R=150A.^o

x	Binding energy (Ry*) (R=150A ^o)
0.10	8.26
0.15	9.54
0.20	10.17
0.25	11.59
0.30	12.86
0.35	13.27
0.40	15.22
0.45	16.11
0.50	17.44
0.55	18.57
0.60	19.22
0.65	20.18
0.70	21.24
0.80	25.86

Table T₅

For finite barrier, barrier height V (Ry*) and band gap energy Eg(Ry*) is given for different constants.

x	V(Ry*)	Eg(Ry*)
0.1	46.292	0.41332
0.2	67.158	0.59745
0.3	88.132	0.77544
0.4	110.246	0.97259
0.5	133.482	1.17345
0.6	157.271	1.38227
0.7	178.486	1.56485
0.8	199.204	1.72395
0.9	209.105	1.89154

4. CONCLUSION

From the above theoretical analysis and evaluation, we come across the following conclusions:

- (i) The concentration plays a significant role in the binding energy of quantum structure.

- (ii) Effective mass approximation with variational and perturbation approaches is useful in the evaluation of binding energy of spherical quantum dot.

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